Rapid Searching of Spectrum Image Databases for Rare Events, or Finding the Needle in the Haystack When You Don't Even Know You're Looking for a Needle!

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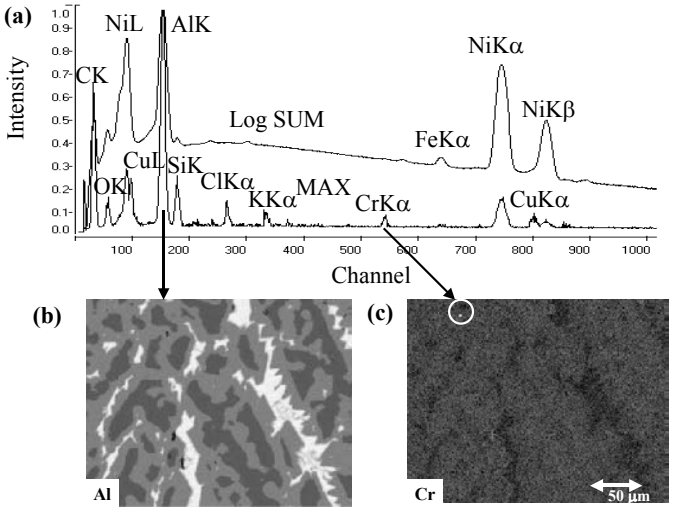
CSTL researchers have developed the *Maximum Pixel Spectrum*, a software tool that enables rapid searching of SEM x-ray spectrum image databases to detect rare features, even if the analyst does not know in advance which elements are present.

Characterization of the microstructure of materials often requires detection of rare features, such as naturally occurring minority/trace phases or unintentional particulate contamination. X-ray mapping in the scanning electron microscope (SEM), a traditional tool for measuring elemental distributions with micrometer to nanometer spatial resolution, has recently been greatly enhanced by the development of x-ray spectrum imaging, in which a complete x-ray spectrum is stored at each pixel location visited by the beam. The silicon drift detector (SDD), described here in FY03 and whose development was aided by NIST Small Business Innovation Research (SBIR) grants, combined with digital signal processing enables x-ray count rates above 100 kHz, permitting recording of useful x-ray spectrum images in 200 s or less. The resulting stream of 200 Mbyte image databases is creating a demand for software tools that are quick and efficient at locating features of interest.

We have developed a software tool within the NIST LISPIX image processing platform that determines the MAXIMUM PIXEL SPECTRUM by finding the maximum value within each energy channel x-y plane and plotting this value versus energy.



(a) SUM SPECTRUM (upper trace, log intensity) and MAXIMUM PIXEL SPECTRUM (lower trace, linear intensity). (b) A major feature (aluminum-containing areas recognized from peaks in the SUM. (c) A rare feature, chromium, detected at a single pixel (inside circle) from the MAXIMUM PIXEL SPECTRUM.

This new function is compared with the SUM SPECTRUM, similarly calculated by adding all values within a plane, as shown in Figure 1(a) for a spectrum image of Raney nickel, a methanation catalyst. Peaks in the SUM SPECTRUM correspond to common features in the x-ray spectrum image, as illustrated in Figure 1(b) where the aluminum-rich phases are highlighted. While these same peaks are found in the MAXIMUM PIXEL SPECTRUM, additional peaks can be recognized that correspond to rare events, down to the single pixel level, shown in Figure 1(c) for a chromium contaminant that appears at a single pixel, or 1/51200 for a 256x200 scan. Note that the rare chromium feature has been found despite being completely unknown to the analyst.

This software tool is available free at http://www.nist.gov/lispix/

The MAXIMUM PIXEL SPECTRUM has had an immediate impact in the microanalysis field. First publicly presented at the SCANNING 04 conference held in Washington in April 2004, the method was immediately adopted by a US manufacturer of microanalysis software systems, appearing in this vendor's system at the Microscopy and Microanalysis Conference in August and in their advertisement in *Microscopy Today* in September 2004. Other vendors are rapidly incorporating the MAXIMUM PIXEL SPECTRUM as a feature in their spectrum imaging software. We anticipate that the combination of SEM SDD x-ray spectrum imaging and derived spectrum image processing tools will have a

broad impact in materials analysis, supporting technology, physical and biological science, and forensic applications. The MAXIMUM PIXEL SPECTRUM and the SUM SPECTRUM are members of a class of transformations known as “derived spectra” to distinguish them from the true spectra recorded in the spectrum image. We plan to investigate additional algorithms for derived spectra to seek software tools that can aid the analyst in other aspects of x-ray spectrum imaging. Other microanalysis spectroscopies, such as electron energy loss and Auger electron, may also benefit from derived spectrum tools.